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Research Article

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Mechanical characteristics, as well as physical-and-chemical properties of the slag-filled concretes, and investigation of the predictive power of the metaheuristic approach

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Abstract: Our article is devoted to development and verification of the metaheuristic optimisation algorithm in the course of selection of the compositional proportions of the slag-filled concretes. The experimental selection of various compositions and working modes, which ensure one and the same fixed level of a basic property, is the very labour-intensive and time-consuming process. This process cannot be feasible in practice in many situations, for example, in the cases, where it is necessary to investigate composite materials with equal indicators of resistance to aggressive environments or with equal share of voids in the certain range of dimensions. There are many similar articles in the scientific literature. Therefore, it is possible to make the conclusion on the topicality of the above-described problem. In our article, we will consider development of the methodology of the automated experimental-and-statistical determination of optimal compositions of the slag-filled concretes. In order to optimise search of local extremums of the complicated functions of the multi-factor analysis, we will utilise the metaheuristic optimisation algorithm, which is based on the concept of the swarm intelligence. Motivation in respect of utilisation of the swarm intelligence algorithm is conditioned by the absence of the educational pattern, within which it is not necessary to establish a certain pattern of learning as it is necessary to do in the neural-network algorithms. In the course of performance of this investigation, we propose this algorithm, as well as procedure of its verification on the basis of the immediate experimental verification.

Keywords: civil engineering; slag-filled concretes; metaheuristic approach

1 Introduction

The majority of investigations in the sphere of the modern constructional materials and components science are devoted to development of the high-quality compositional materials, which would be in accordance with their destination in the best possible way. In this regard, such compositional materials are usually referred to as the high-performance materials [1–3]. Both high-strength concrete, which is intended for the bridge structures, and the rapid-hardening low-strength mortar, which is intended for the short-term reinforcement of the relevant materials, can be included to the category of such materials.

This appropriation imposes the certain set of requirements in respect of: the criteria of quality of the relevant material at the various stages of its production life; characteristics of the structure; technological and performance characteristics; criteria for persistence, level of which determines the entire working life of the relevant structure (particularly, in the case of operation in the severe environmental conditions, in the aggressive environments, in the conditions of low and/or high temperatures). In addition, there exist the requirements in respect of: reliability; security of properties in the systems, failures of which would cause impermissible consequences; environmental criteria in respect of the relevant "soundness" of technology; waste utilisation; cost-effective use of resources, etc. Particularly, the concept of sustainable development [4] puts forward requirements in respect of the assurance of persistence and durability of concretes. Solving of this problem would make it possible to: reduce CO_2 emissions in the course of cement production; decrease consumption of natural aggregates from the existing sources, which are al-

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most exhausted already; mitigate the problem of removal of the concrete of the destroyed structures; as well as to decrease expenses on repairs [2].

As of today, manufacturing companies are forced to develop new high-technology products in record-breaking time. At the same time, they must increase both quality of these products, and efficiency of the relevant technological processes in a narrow and in a broader sense. The latter statement means that despite of the fact that increase of the durability is achieved, as a rule, at the expense of high "initial" cost of the material as such, however, this process would make it possible to decrease "total" costs. That is, this process would be efficient for the entire system, which contains such material. Therefore, such high-quality material would be the competitive product.

In this case, it is understood that it is necessary to ensure efficiency of the entire life of such material, "from birth to death" (beginning from the first idea, through investigation, designing, and production, in the course of utilisation of this material through the stage of its degradation up to the stage of disposition). This statement complies with the modern philosophy of quality: it is necessary to assure quality of the product from the very beginning (idea, project).

Similar problems occur in many branches of economy, where it is necessary to develop chemical compounds with complicated compositions provided that such compounds must comply with many conflicting requirements. For example, neural networks have found widespread application already in the processes of development of the complicated molecules of various pharmaceutical products. This fact is conditioned by the necessity of searching the optima among many alternatives. In the course of accumulation of the vast majority of the immediate data in respect of the physical-and-chemical properties, biological activity, spectra, and reactive capacity of various organic compounds, the problem of generalisation and statistical processing of these data has become very topical. Solving of this problem would make it possible to develop methods of forecasting properties of new chemical compounds, as well as to begin the target-specific molecular design of the compounds, which would have the predetermined set of properties. In the last few years, several hundred statistical approaches and methods of the computer-aided learning are actively developed and used. A certain group of methods (which are usually referred to as the "artificial neural networks", "computational neural networks", or simply "neural networks") plays the main and ever-increasing role among all these approaches and methods.

In addition, it is also possible to mention article [5] and to pay attention to article [6]. Within the latter article, complexity of optimisation of the composition, which must comply with the conflicting requirements, has resulted in development of the relevant mathematical model and the algorithm, which ensures optimisation of this composition in accordance with the predetermined operational parameters and price. The algorithm, which is described in this article, makes it possible to substantiate and to select optimum reagents at each stage and, consequently, to recommend them for subsequent investigation. The whole purpose of this experiment was connected with the necessity to determine the optimum relationship of the original reagents. In addition, this article describes process of selection of the most efficient emulsifying agent (type, concentration) for the required combination of components through decreasing proportion of this emulsifying agent in the final solution and, therefore, preparation of the technological agent, which would have the desired properties [7, 8].

In our article, we would like to develop similar approach in order to forecast properties of the slag-filled concretes. Of course, concretes (even if they are multicomponent/blended concretes) are much more simple compounds as compared with the pharmaceutical products; therefore, it is possible to simplify this algorithm essentially. However, the most substantial components of this approach (search, classification, and sorting of the local minimums of the integral function in the course of the multi-factor analysis, which takes into consideration all properties of the compounds under investigation) cannot be simplified, and they will remain unchanged, therefore they must be performed in all entirety. In the case of more simple function in the course of the multi-factor analysis, it would be possible to forget all complexities, which are connected with simulation of behaviour of big quantity of neurons. Therefore, it would be possible to make search with the help of the algorithms of the swarm intelligence or with the help of the evolutionary algorithms (instead of simulation of the neural network). Then, there is the question as follows: why it is not possible to perform direct experiments for the simple concretes? There is the answer, of course. As concerns the sphere of constructional materials science, any experiment (being the main source of information), as a rule, is the very labour-intensive and time-consuming process (great cost of materials, as well as duration of the structure formation and destruction processes). First of all, it is connected with duration of the destruction processes. Indeed, how it is possible to obtain the prompt answer to the following question: whether a concrete of a certain composition would have its carrying properties during a prolonged period of time in any aggressive environment, for example, in the conditions of the seawater? There exist many assumptions, which make it possible to estimate the resistance of concretes to chemical attacks, as well as their mechanical strength, however, they are hypothetical assumptions to a certain degree and they cannot give the relevant answer as the result of the immediate experiment, but such experiment can require many time. It is understood that in order to obtain prompt answers in these conditions, it would be necessary to develop methods of the experimental-and-statistical simulation. Therefore, an experiment and simulation are two components of the joint system, which ensures optimisation of the formulation-and-technological solutions.

It is possible to state that the approach, which we propose to apply, is the kind of the experimental-and-statistical simulation. It is a certain combination of presentations, methods, and algorithms, which connects mathematical planning of experiment, regression analysis, and other facilities of the applied statistics with the meaningful analysis of models and which is intended to the most comprehensive extraction of information from the experimental data in respect of the object/system under investigation [9–11]. Such combination is necessary in order to ensure utilisation of these data and simulate a composition of the building material with the predetermined properties without performance of the full-scale experiment. This package of facilities for investigation/simulation includes four main modules of the interconnected actions.

1. Determination and substantiated selection of the experiment conditions, that is, "the advanced planning" [12] and "metrisation" [13] of the experiment. Selection (on the basis of the system approach) of those factors, which can be varied in the course of this experiment (selection of the controlled input factors, levels of which can be predetermined or fixed), as well as selection of those criteria, which can be measured (selection of the output factors, responses, properties of the object). At the same time, it is necessary to determine the ranges of such variation taking into account the physical-and-chemical properties, technological parameters, as well as other a-priori knowledge and various data in respect of this experiment. All these data must be agreed with the methodological and metrological features of the relevant object, as well as with the instrumental possibilities of the entire investigation.
2. Planning of the optimum multi-factor experiment [9, 12, 13]. At this stage, it is necessary to analyse and take into consideration the following parameters: structure of the vector of various factors; form of the regression model, which would be rational for the relevant problem; obligatory experiments (at the certain combinations of levels of the relevant factors), which must be predetermined "by the concrete technologist"; as well as "the prohibited" zones of the factor space [13].
3. Development of the regression models in accordance with the experimental data. These models must be cleared from the statistically insignificant effects. In addition, these models must be recognised as the models, which are adequate to the results of the relevant experiment (in accordance with the accepted risk or the accepted error level). In a certain number of situations, it is allowed to utilise the algorithm "with the generated error of this experiment" [14].
4. Solving of the scientific and technological problems in respect of each specific experimental-and-statistical model, as well as in respect of the entire package of these models [9, 13] with the help of the special facilities of visualisation (with subsequent convolution of the multi-factor functions into the small-dimensional functions, which can be represented as graphs, as diagrams "of the potential landscapes", and so on.). These problems are the problems of: analysis, interpretation, optimisation; determination of the permissible and optimum solutions; minimisation of resources; estimation of role of various factors; estimation of confidence intervals for engineering recommendations, etc.

In our article, we will consider development of the methodology for the automated experimental-and-statistical determination of optimal compositions of the slag-filled concretes. In order to optimise search of local extremums of the complicated functions in the course of the multi-factor analysis, we will utilise the metaheuristic optimisation algorithm, which is based on the concept of the swarm intelligence. Slag-filled concrete is the concrete, which complies with the special combinations of requirements in respect of the productivity and smoothness and which is manufactured with utilisation of unusual components of the concrete, as well as with certain variations in respect of the practice of mixing, installation, and hardening of the concrete. Dosing of the concrete mixtures for the slag-filled concretes includes three stages: (1) selection of the suitable components; (2) determination of quantities of various components for production of the concrete, which would be cost-effective, however, which would achieve the desired characteristics, as well as (3) painstaking quality control of each process of the concrete production [15]. At the stage (1) combination of relevant materials is determined on the basis of the desired characteristics, availability of materials, and their prices. Stage (2) is interconnected with the stage (1), because of quantity of each material, which was selected at the stage (1), is determined in order to ensure achievement of the desired characteristics in the most cost-efficient manner. Proportion of the mixture, which was determined at the stage (2), will be additionally checked with utilisation of the trial concrete mixes in order to be sure that proportion of the mixture complies with both the desired characteristics, and the cost-effective aspect. Stage (3) includes subsequent important operations: proper monitoring of smoothness of raw materials, dosing, mixing, transportation, installation, vibromechanical treatment, and hardening of the concrete, including tests of the hardened concrete [15]. Good proportion of the mixture would result in the satisfactory quality of the concrete, which would have all desired characteristics, as well as would minimise quantity of the trial concrete mixes [16].

Taking into consideration the importance of achievement of the correct proportion of the concrete mixture, we will concentrate our attention in this article on the second stage, that is, on determination of quantity of various components. Difference between compositions of the slag-filled concrete and usual concrete is connected with the fact that the slag-filled concrete contains certain additional materials and chemical additives (slag as such, as well as other compensating additives). At the same time, the slag-filled concrete contains the main components of the usual concrete (that is, ordinary Portland-cement, water, fine aggregates, and coarse aggregates) [17, 18]. However, there is no any uniform or unique composition for such concretes; therefore, selection of the optimum composition of such concrete will be an original problem every time [19, 20]. In the absence of the generalised systematic method of composition of the concrete mixtures, trial concrete mixes play the main role in the process of finding suitable proportion of the concrete composition, which would have the desired specific characteristics [21]. Despite of the fact that several methods of designing were already developed, there is no any generalised systemic method for dosing the composition for an arbitrary concrete mixture until now (and certainly, there is no method for such complicated compositions as the slag-filled concretes). In these latter days, there are many publications, which are devoted to various attempts to develop any such generalised methodology [16, 22–24]. Many methods on the basis of the artificial intelligence have been already developed in order to forecast quality of the concrete and ensure optimisation in the course of the multi-factor analysis of the experimental-and-statistical data. However, algorithms of the metaheuristic optimisation can be of special interest [25–27]. In our article, we will use a certain variation of the swarm intelligence algorithm in order to search local and global extremums in the course of the multi-factor analysis of the experimental-and-statistical data. Motivation in respect of utilisation of the swarm intelligence algorithm is conditioned by the absence of any educational pattern, within which it is not necessary to establish a certain pattern of learning as it is necessary to do in the neural-network algorithms. Therefore, this method prevents any forced fitting of the experimental data in accordance with the usual equations for calculation of the concrete mixture or in accordance with any other function. This algorithm is the algorithm of the external nature in respect of the analysed data. Therefore, it can be adapted to the data of any nature with the help of the inessential adjustments. Moreover, in the case of addition of any new data to the database, learning of the algorithm is not required. As compared with other popular algorithms of clusterisation (such as fuzzy C-average, K-average, and spectral clusters, fuzzy ART-clusterisation), it is not necessary to state quantity of clusters in our case.

2 Materials and methods

2.1 The materials, which are utilized in practice

In order to check the proposed metaheuristic algorithm in the course of estimating the proportion of the slag-filled concrete mixture, we have collected the special database, which included the data of relevant experiments. Results in respect of 79 proportions of the slag-filled concrete mixtures were collected in the database, which was provided by the company that produces the premixed dry concretes. The materials, which were used in the slag-filled concrete, were as follows: ordinary Portland-cement, F Class slag, water, river sand, coarse aggregates (maximum dimension of particles: 20 mm), and superplasticizers on the basis of the polycarboxylate ethers (PCE). All these tests were performed with the help of the cubic samples (dimensions: 10 cm × 10 cm × 10 cm), which were manufactured in accordance with the procedures of the relevant standard (MS EN 12390). Table 1 presents the materials, which are utilized in practice, as well as values of the 7th day compressive strength and 28th day compressive strength.

Table 1: Range of materials and compressive strength in the database of the fly-ash high-performance concretes

Materials	Unit of meas-t	Minimum	Maximum	Average	Standard deviation
Ordinary Portland cement	kg/m^3	364	702	507.95	75.53
Fly ash	kg/m^3	0	272	127.26	67.06
Water	kg/m^3	118	175	148.13	11.70
Fine aggregates	kg/m^3	611	764	670.69	42.57
Coarse aggregates	kg/m^3	917	1,086	968.63	42.69
Superplasticizer	kg/m^3	3.33	17.165	7.135	2.94
7th day compressive strength	MPa	46.17	91.5	65.72	8.71
28th day compressive strength	MPa	63.17	106	80.38	6.89

2.2 The algorithm of the metaheuristic optimisation

Let us assume that $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is the target function, which must be minimised, S is the quantity of particles within the swarm. Let us assume that each of these particles is characterised by its individual value of the coordinate $\mathbf{x_i} \in \mathbb{R}^n$ within the space of solutions, as well as by its individual value of the velocity $\mathbf{v}_i \in \mathbb{R}^n$. Let us also assume that $\mathbf{p}_i$ is the best known position of the particle i, while $\mathbf{g}$ is the best known state of the entire swarm. Then, general presentation of the swarm method is as follows.

- For each particle $i = 1, \ldots, S$ it is necessary to do the following:
  - To generate initial position of the particle with the help of the arbitrary vector $x_i \sim U(\mathbf{b_{lo}}, \mathbf{b_{up}})$, which would have the multivariate uniform distribution. In this case, $\mathbf{b_{lo}}$ and $\mathbf{b_{up}}$ would be the lower and the upper boundaries of the space of solutions, respectively.
  - To ensure that the best known position of this particle will be determined in accordance with its initial value: $\mathbf{p}_i \leftarrow x_i$.
  - If $(f(\mathbf{p}_i) < f(\mathbf{g}))$, then it is necessary to renew the best known state of the swarm as follows: $\mathbf{g} \leftarrow \mathbf{p}_i$.
  - To ensure that this particle will be determined in accordance with its value of velocity: $\mathbf{v}_i \sim U(\text{-}(\mathbf{b}_{up}\text{-}\mathbf{b}_{lo}), (\mathbf{b}_{up}\text{-}\mathbf{b}_{lo}))$.
- It is necessary to repeat these operations until the moment, when the stopping criterion would be performed (for example, until the moment, when the predetermined quantity of iterations or the necessary value of the target function would be achieved):
- For each particle $i = 1, \ldots, S$ it is necessary to do the following:
  - To generate arbitrary vectors $\mathbf{r}_p, \mathbf{r}_g \sim U(0,1)$.
  - To renew value of velocity of the particle: $\mathbf{v}_i \leftarrow \omega\, \mathbf{v}_i + \varphi_p\, \mathbf{r}_p \times (\mathbf{p}_i\text{-}x_i) + \varphi_g\, \mathbf{r}_g \times (\mathbf{g}\text{-}x_i)$, where "×" operation means the component-wise multiplication.
  - To renew value of position of the particle with the help of operation of transfer $\mathbf{x_i}$ to the vector of velocity: $\mathbf{x_i} \leftarrow x_i + \mathbf{v}_i$. It is worth to note that this operation is to be performed regardless of the improvement of value of the target function.
  - If $(f(x_i) < f(\mathbf{p}_i))$, then it is necessary to do the following:
    - To renew value of the best known position of the particle: $\mathbf{p}_i \leftarrow \mathbf{x_i}$.
    - If $(f(\mathbf{p}_i) < f(\mathbf{g}))$, then it is necessary to renew the best known state of the entire swarm: $\mathbf{g} \leftarrow \mathbf{p}_i$.
  - Now value of $\mathbf{g}$ contains the best solution as compared with all other solutions, which were already found.

Parameters ω, φ_p, and φ_g must be selected with the help of computations. These parameters determine behaviour and efficiency of the entire method. These parameters form the subject-matter of many investigations. Pedersen *et al.* have proposed the simple and efficient way to select parameters of this method. Therefore, we will follow propositions of their articles [28, 29] to a considerable extent. In addition, these authors have performed the numerical experiments with various optimisation problems and parameters. Methodology of selection of these parameters is referred to as the "meta-optimisation", because of an-

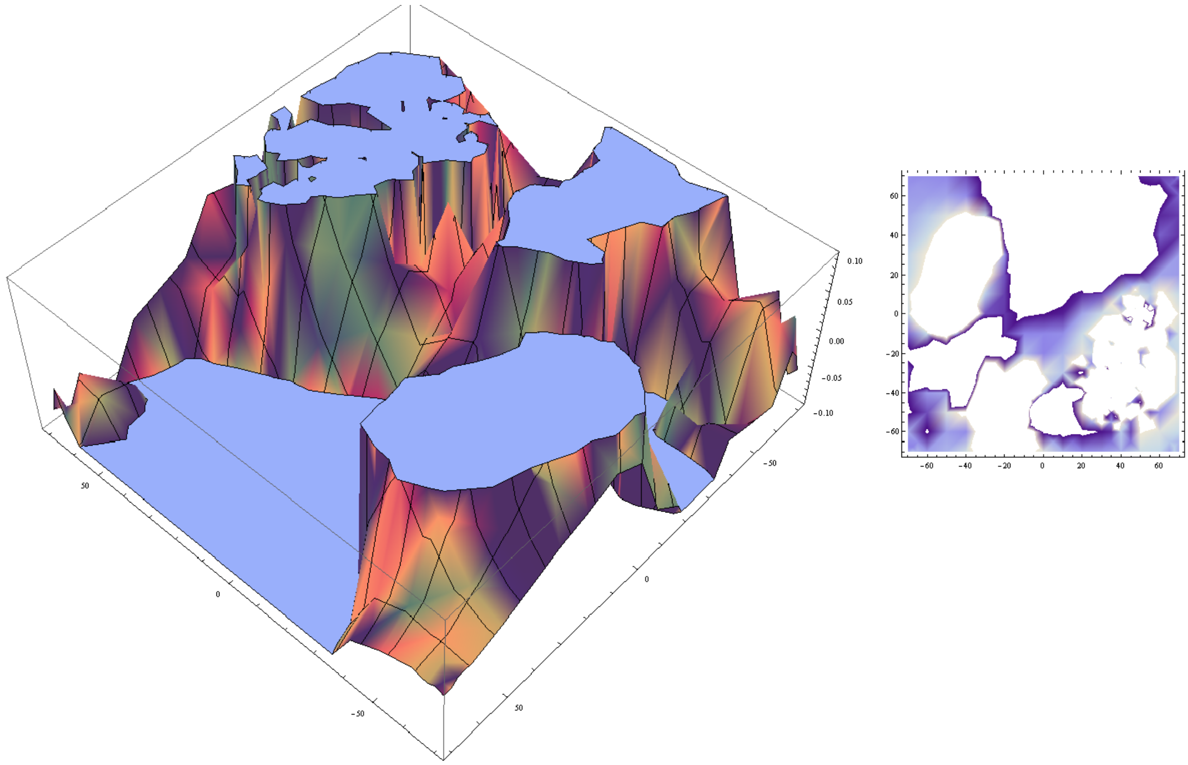

Figure 1: The adaptational landscape, which was constructed on the basis of reference points of the experimental data. The left section presents convolution to the three-dimensional image. The right section presents the space for determination of the function, which would comply with the target indicators of the concrete strength, which were prescribed at the input of the metaheuristic algorithm.

Table 2: The proposed proportions of the composition, which were obtained on the basis of the metaheuristic optimisation.

Desired 7th day/28th day compressive strengths (MPa)	Tolerances (%)	Cement (kg/m^3)	Fly ash (kg/m^3)	Water (kg/m^3)	Sand (kg/m^3)	Granite (kg/m^3)	Superplasticizer (l/m^3)	Estimated 7th day/ 28th day compressive strengths (MPa)
55/65	±5/±10	390	213	142.125	676.5	981	5	51.00/68.16
58/70	±5/±5	470	130	169.11	664	996	3.86	56.88/70.72
60/75	±5/±10	470.24	136.24	146.92	703.41	971.71	6.796	57.31/75.85
68/80	±5/±10	498.5	189.5	140.583	624	936.25	11.293	66.37/81.33
70/85	±5/±5	573	112.57	145.90	644.29	943.71	9.54	71.85/85.10

other optimisation algorithm is utilised in order to "adjust" parameters of the entire swarm. The input parameters of the swarm intelligence algorithm with the best productivity do not correspond to the main principles, which are described in the scientific literature. Therefore, these parameters often ensure satisfactory results of optimisation for the simple situations only. It is possible to read description of implementation of these parameters in the SwarmOps open-source library [30].

3 Results and discussion

In accordance with the database, which contains the characteristics that are presented in Table 1, the proposed metaheuristic algorithm for estimating the proportion of the slag-filled concrete composition was used in the course of estimating proportions of the composition for the desired values of the 28th day compressive strength (these desired values were as follows: 65, 70, 75, 80, and 85 MPa with tolerances ±5%). In addition, we have attempted to demonstrate universality of the proposed fuzzy model on the basis of the metaheuristic algorithm, which is capable to predict more than one criterion of efficiency. Therefore,

Table 3: Comparison of the predicted and experimental results.

Desired 7th day/28th day compressive strengths (MPa)	Predicted results (MPa)	Experimental results (MPa)	Errors (%)
55/65	51.00/68.16	57.80/71.40	+11.76/4-4.76%
58/70	56.88/70.72	50.53/72.75	−12.6/+2.87%
60/75	57.31/75.85	57.23/80.45	−0.14/+6.07%
68/80	66.37/81.33	75.30/82.70	+11.9/+1.68%
70/85	71.85/85.10	68.24/87.10	−5.29/+2.35%

we have also determined the second criterion of efficiency, that is, the 7th day compressive strength with tolerances ±5% or ±10% (depending on the suitability of the relevant tolerance in order to determine such proportion of the mixture, which would correspond to both criteria of efficiency). Table 2 presents results of this attempt.

Figure 2 presents the three-dimensional image of the multidimensional function (in the adaptational landscape), within which the proposed metaheuristic algorithm performs search of the optima (following convolution of the dimensionality of this function)

Figure 2 and Table 3 present comparison of the experimental and theoretical attempts

The forecasted results of the metaheuristic optimisation in the course of estimating the proportion of the slag-filled concrete mixture, which are presented in Table 2, have been used in the experimental work with the purposes of verification. In order to ensure reproducibility of results, we have used the concrete samples with the same dimensions, that is, we have used the cubes with the 10 cm length of edges. It is important to emphasize that the experimental work has been performed at another production shop, where the fine and coarse filling agents for the concrete mixtures differ from the samples, which were manufactured for the initial database (it is the obvious restriction of the entire our investigation). However, the Portland-cement, slag, and superplasticizer were the same. Table 3 presents comparison of the desired, predicted, and experimental results. Each experimental result is the average value for three samples. It is obvious that all experimental results for the 28th day compressive strength exceed the predicted results (with errors from 1.68% up to 6.07%). Errors of results for the 7th day compressive strength exceed the errors for the 28th day compressive strength; however, all these errors are lower than 12.6%.

Later on, we have performed the statistical analysis between the predicted results and experimental results. We have determined values of the root-mean-square errors at the level of 4.7 MPa, as well as value of the coefficient of determination (R^2) at the level of 0.996. These results confirm

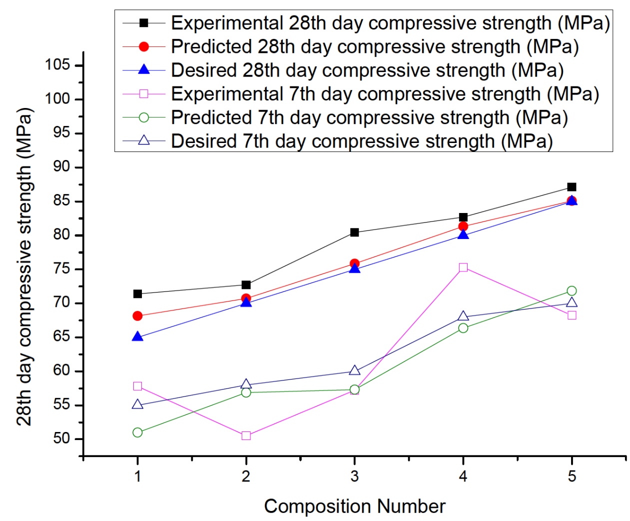

Figure 2: Comparison of the desired, predicted, and experimental results.

accuracy of the metaheuristic optimisation in the course of estimating and forecasting proportions of the slag-filled concrete composition. In addition, these results demonstrate that the metaheuristic optimization, which is proposed for estimating the proportion of the slag-filled concrete composition, is both useful and reliable tool for the new approach to the procedure of designing various new compositions. In the situations, where the concrete mixture would be prepared in accordance with the predicted proportion with utilisation of the standard procedure, it would be possible to achieve the desired characteristics of the concrete.

4 Conclusions

This article describes discussion of the metaheuristic optimisation on the basis of the swarm intelligence algorithm in the course of estimating the proportion of the slag-filled concrete composition with the predetermined characteristics in accordance with the experimental data. Thus, we develop the model, which obtains the desired characteristics of the concrete from the end-user from the very beginning. Then this model selects the data, characteristics of which are close to the required characteristics, and constructs the multidimensional space, within which it is possible to define the multidimensional polynomial function, for which relevant adaptation landscape is defined on the basis of the reference points of the experimental data. Later on, the metaheuristic swarm intelligence analyses this multidimensional landscape in order to organise search of extremums. Then this metaheuristic swarm intelligence finds global and local optimums, classifies them, and, at last, estimates the proportion of the concrete mixture. The calculated proportion of the mixture, which was proposed by this model, was confirmed by the experimental data in respect of the slag-filled concrete. It was established that the predicted results are in good correspondence with the experimental results: maximum errors of forecasting are equal to 12.6% (for the 7th day compressive strength) and 6.07% (for the 28th day compressive strength). In addition, it was demonstrated that this model is capable to estimate proportions of the mixture with various components. At the same time, the model can to reveal potential emissions. This advantage would help to prevent utilisation of the potential emissions in the course of estimating proportion of the concrete mixture. However, utilisation of this model will be restricted, if volume of the relevant database will be small due to the absence of the data, which can define the set of the certain characteristics of the concrete. Another restriction of this model is connected with the fact that it cannot take into account the experimental data, which do not correspond to the predetermined initial data (for example, if the experimental reference point with incomplete/absent data was defined). Of course, it is not a critical restriction; however, we have already planned subsequent investigations in order to ensure utilisation of this model in the cases of absence of the input data.

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